A Phase-Free Quantum Monte Carlo Method for the Nuclear Shell Model

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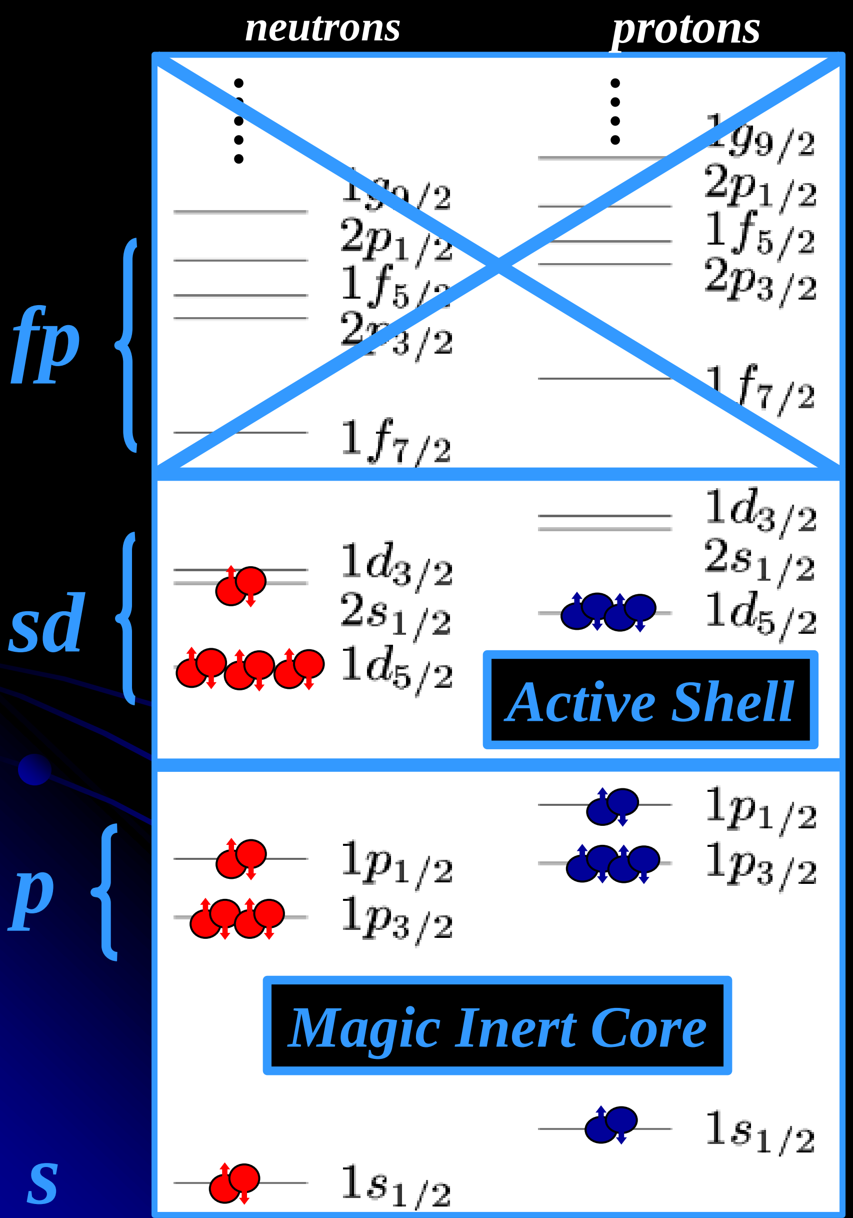
The Nuclear Shell Model

Mean-field approximation



ex: ^{28}Mg

Residual interaction

Two-body effective interaction

e.g. *G*-matrix

Configuration interaction

Diagonalization of the Hamiltonian matrix in the independent-nucleon basis

Spectroscopy, Transition probabilities, electromagnetic moments…

Motivations

Exponential growth of the size of the many-body basis with the nucleon number and / or the number of valence levels

Quantum Monte Carlo methods could be an alternative to the direct diagonalization of the Hamiltonian

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Shell Model Monte Carlo

S.E. Koonin, D.J. Dean, K. Langanke
Phys. Rept. 278,1 (1997)

- ✓ *Ground-state properties*
- ✓ *Thermodynamic properties*
- ✗ *Spectroscopy*
- ✗ *Sign problem*

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- ✗ *Spectroscopy*
- ✗ *Sign problem*

Objective

An alternative to the diagonalization to obtain the "yrast spectroscopy" with a controlled sign problem

QMC: *the fundamentals*

- ***Correlated state*** $|\Psi\rangle$
- ***Slater determinant*** $|\Phi\rangle$

Configuration Interaction

$$|\Psi\rangle = \sum_{\Phi} A_{\Phi} |\Phi\rangle \quad \textbf{\textit{with}} \; |\phi_i\rangle = |n_i l_i j_i m_i \tau_i\rangle$$

***Quantum Monte Carlo* (QMC)**

$$|\Psi\rangle = \int_{\Phi} \mathfrak{D}\Phi \, A(\Phi) |\Phi\rangle \quad \textbf{\textit{with any}} \; |\phi_i\rangle$$

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Real & positive

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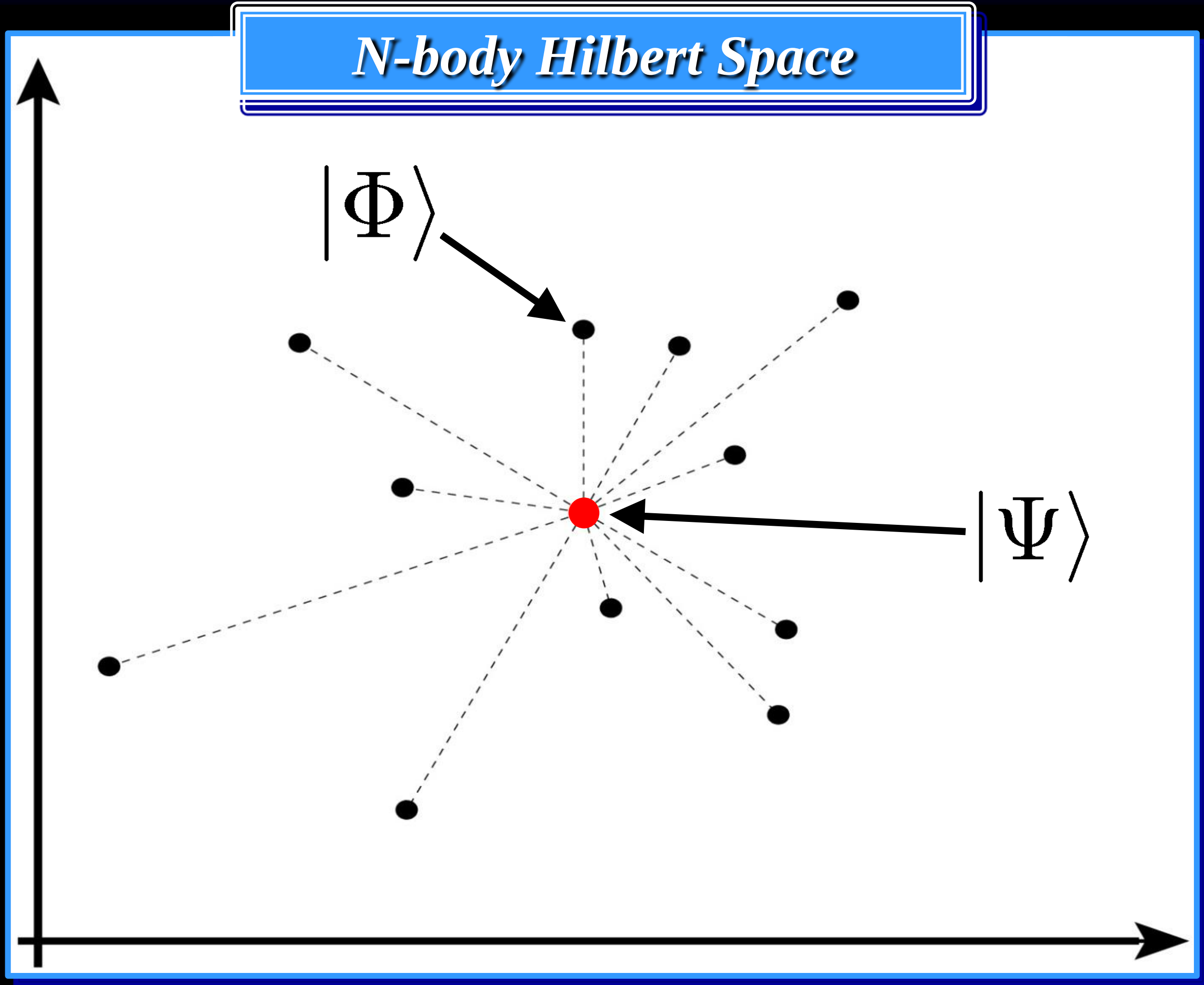

Quantum Monte Carlo **(QMC)**

$$|\Psi\rangle = \int_{\Phi} \mathfrak{D}\Phi \boxed{A(\Phi)} |\Phi\rangle$$

Real & positive

Reformulation of the exact state as an average of independent-particle states

$$|\Psi\rangle \propto \mathbb{E}\left[|\Phi\rangle\right]$$

Imaginary-Time Propagation

$$|\Psi_g\rangle \underset{\tau\to\infty}{\propto} \mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle$$

Projects any wavefunction onto the ground state having the same symmetries

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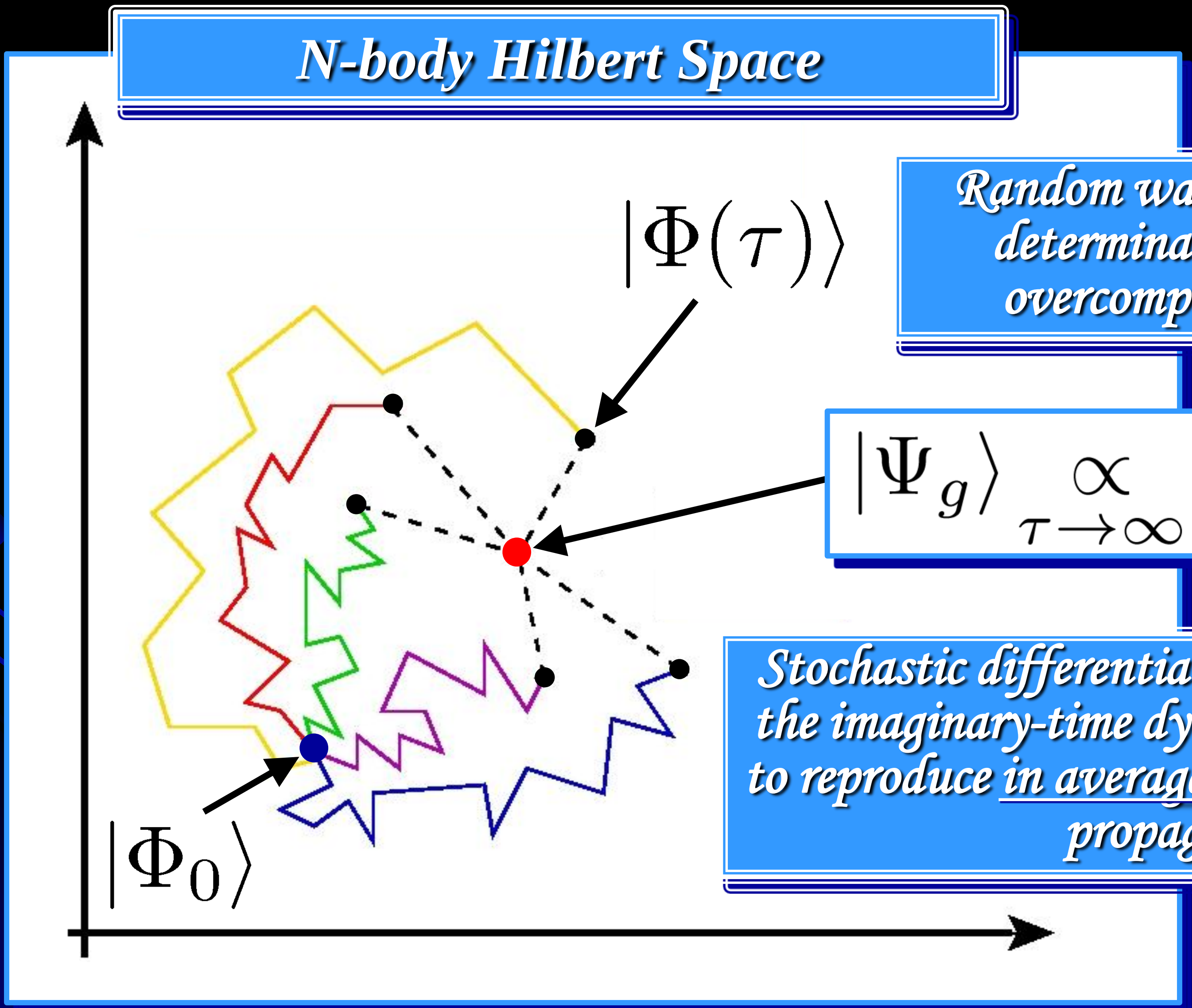
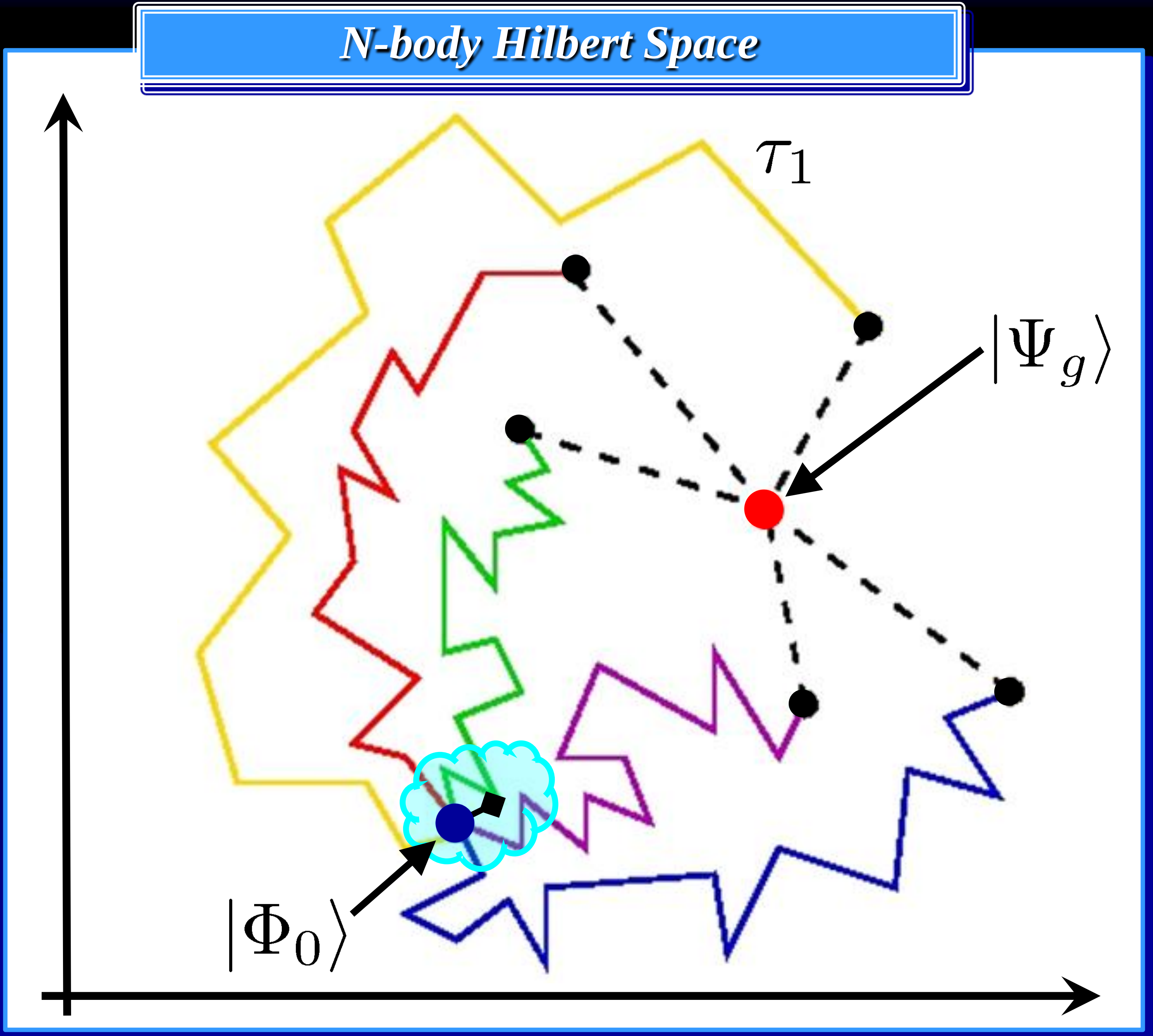


Random walk of Slater determinants in the overcomplete basis

$$|\Psi_g\rangle \underset{\tau\to\infty}{\propto} \mathbb{E}\big[|\Phi(\tau)\rangle\big]$$

Stochastic differential equations governing the imaginary-time dynamics of the orbitals to reproduce <u>in average</u> the exact many-body propagation

QMC : *Importance of the initial state*



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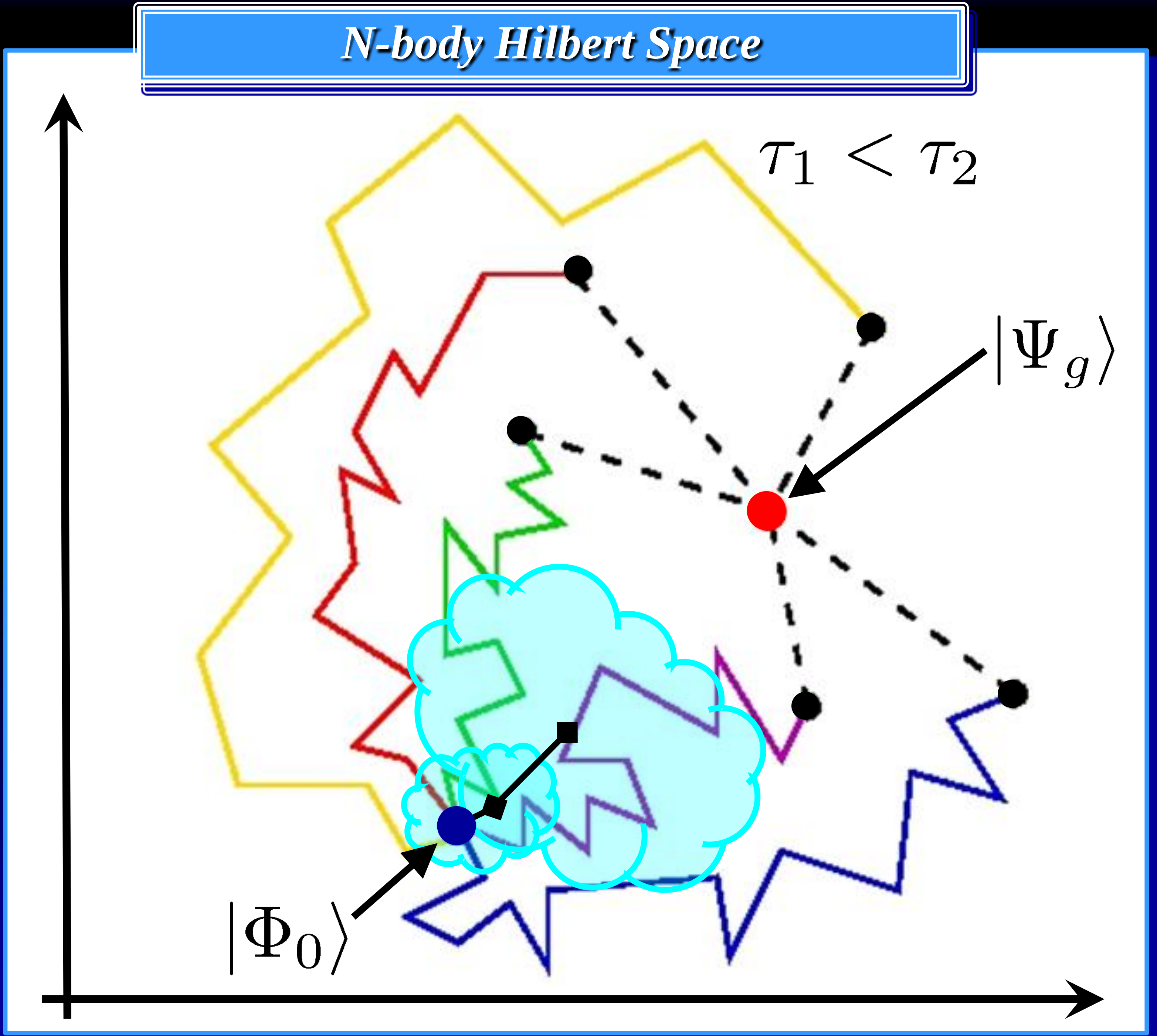

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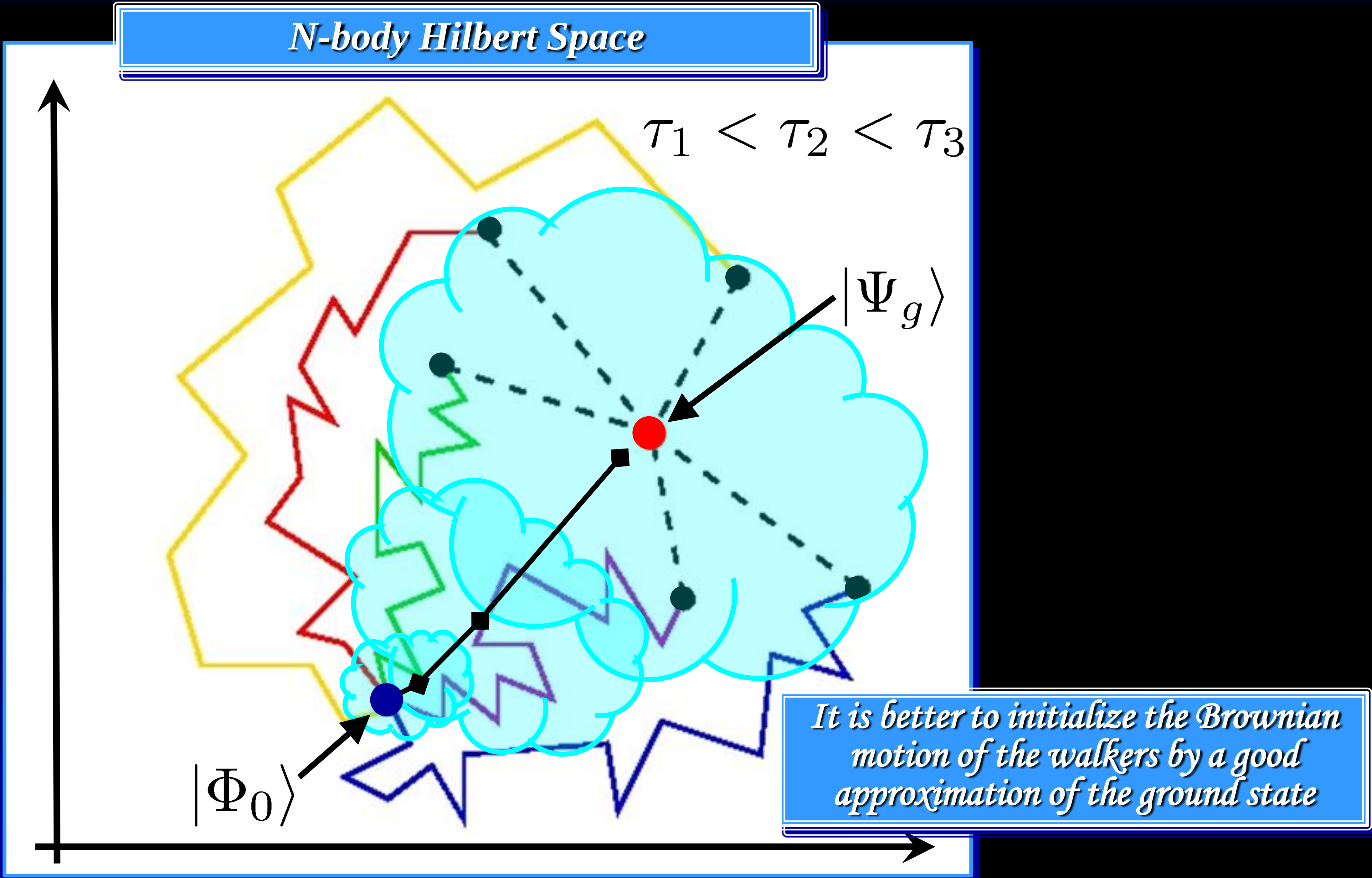


Choice of the initial state

Variational method with projection on the symmetries before variation

Projected Hartree-Fock method **(PHF)**

$$\delta E_J = \delta \left[\frac{\langle \Psi_{JM} | \hat{H} | \Psi_{JM} \rangle}{\langle \Psi_{JM} | \Psi_{JM} \rangle} \right] = 0 \; ; \; |\Psi_{JM}\rangle = \sum_{K=-J}^{J} C_K^{(J)} \hat{P}^J_{MK} |\Phi_0\rangle$$

- $|\Phi_0\rangle$ ***and the*** $C_K^{(J)}$***'s are determined by minimizing the projected energy*** E_J
- $\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int \mathrm{d}\Omega D^{J*}_{MK}(\Omega) \hat{R}(\Omega)$ ***Projector onto a good angular momentum J***

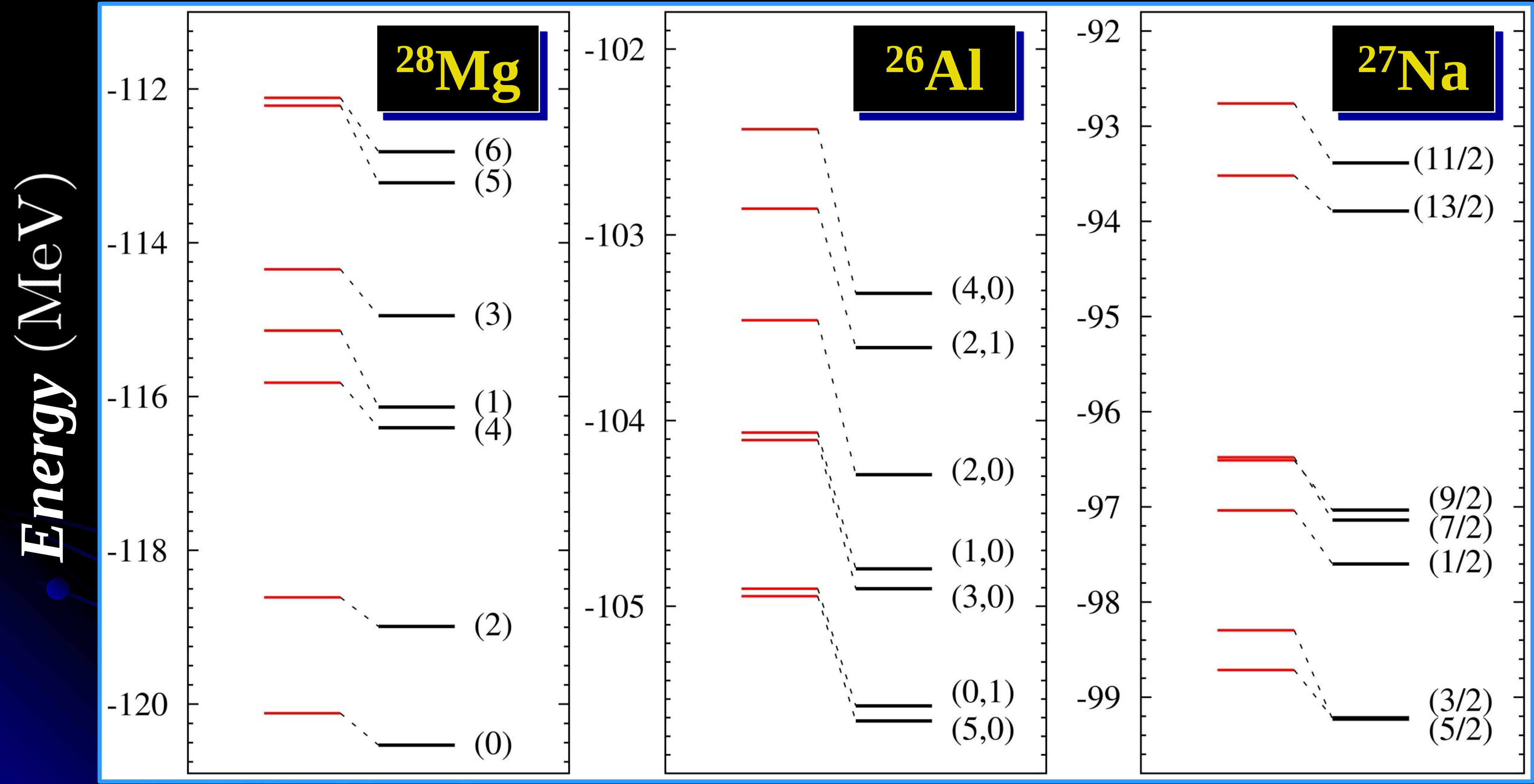
→ **VAMPIR** ***method without pairing and with*** $|\Phi_0\rangle = |\Phi_0^p\rangle \otimes |\Phi_0^n\rangle$

Variation After Mean-field Projection In Realistic model space

K.W. Schmid *et al.*, *PRC* 29,291 (1984)

T. Hjelt *et al.*, *EPJA* 7,2,201 (1995)

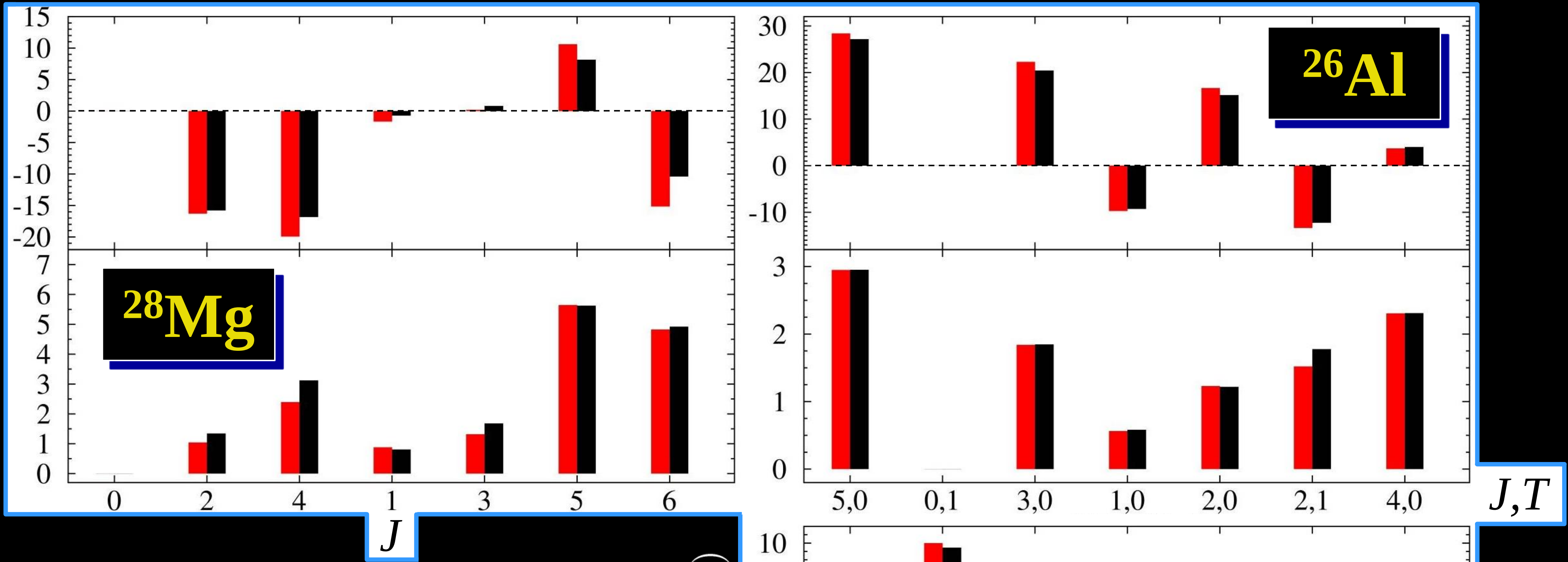
PHF *Results*: *Spectra*

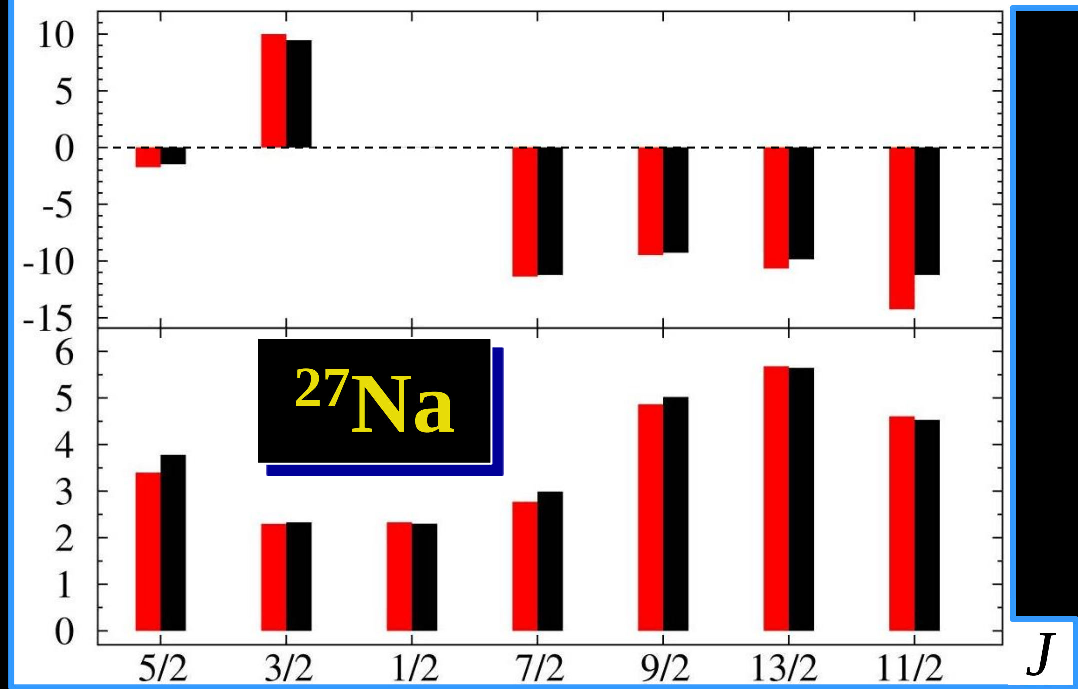


- *PHF*
- *Exact* (J) *or* (J,T)

- *Effective interaction*: USD
  - H. Wildenthal, *PPNP* 11,5 (1984)
  - A. Brown, H. Wildenthal, *ARNPS* 38,29 (1988)
- *Exact results from the code* ANTOINE
  - E. Caurier *et al.*, *Acta Pol.* 30,705 (1999)
  - E. Caurier *et al.*, *Rev. Mod. Phys.* 77,2 (2005)

PHF *Results*: *Moments*





- *PHF*
- *Exact*

Effective charges

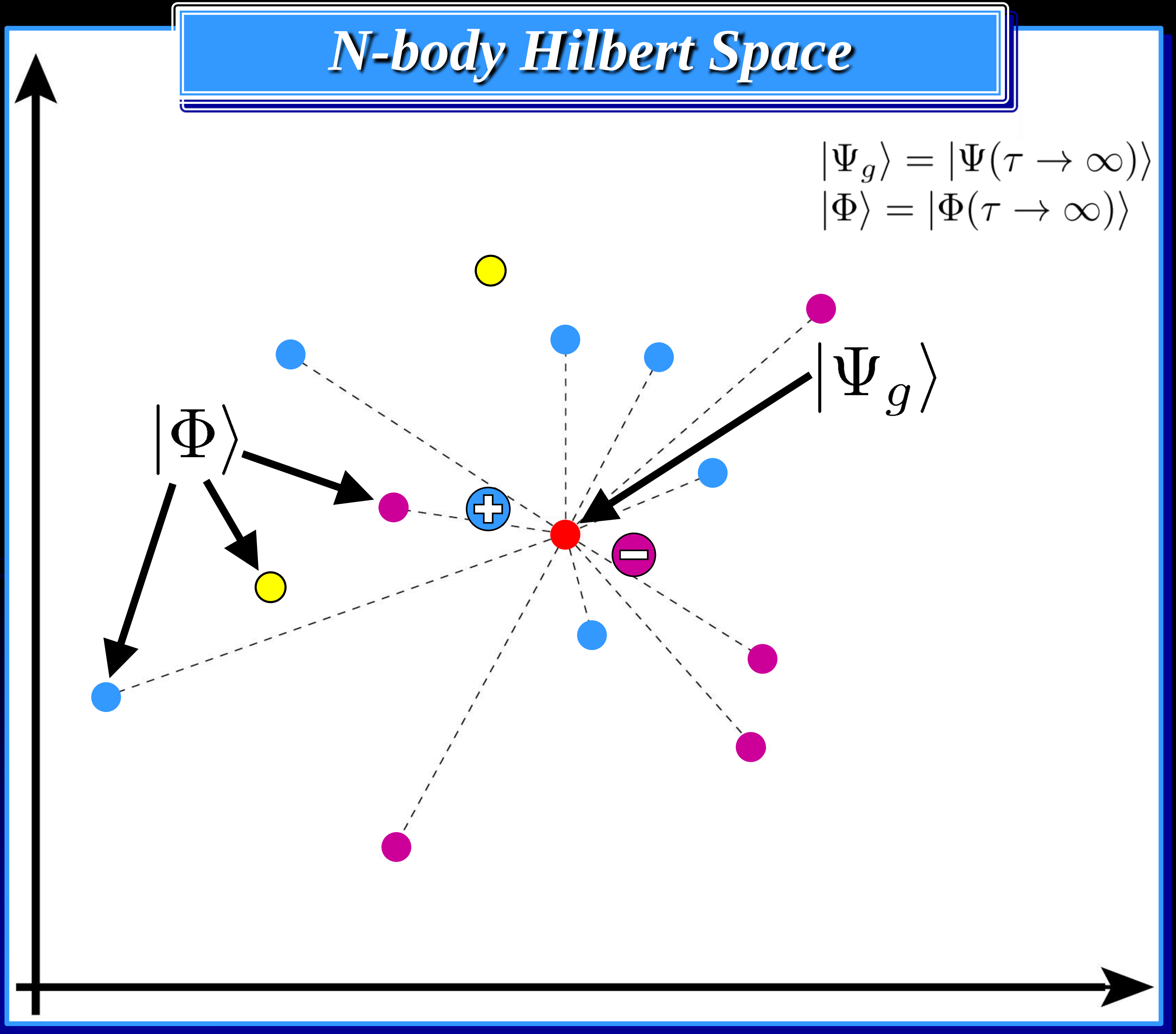
$e_n = 0.49e\ ;\ e_p = 1.29e$

Effective g-factors

$g_n^s = -3.875\ ;\ g_n^l = 0.036$

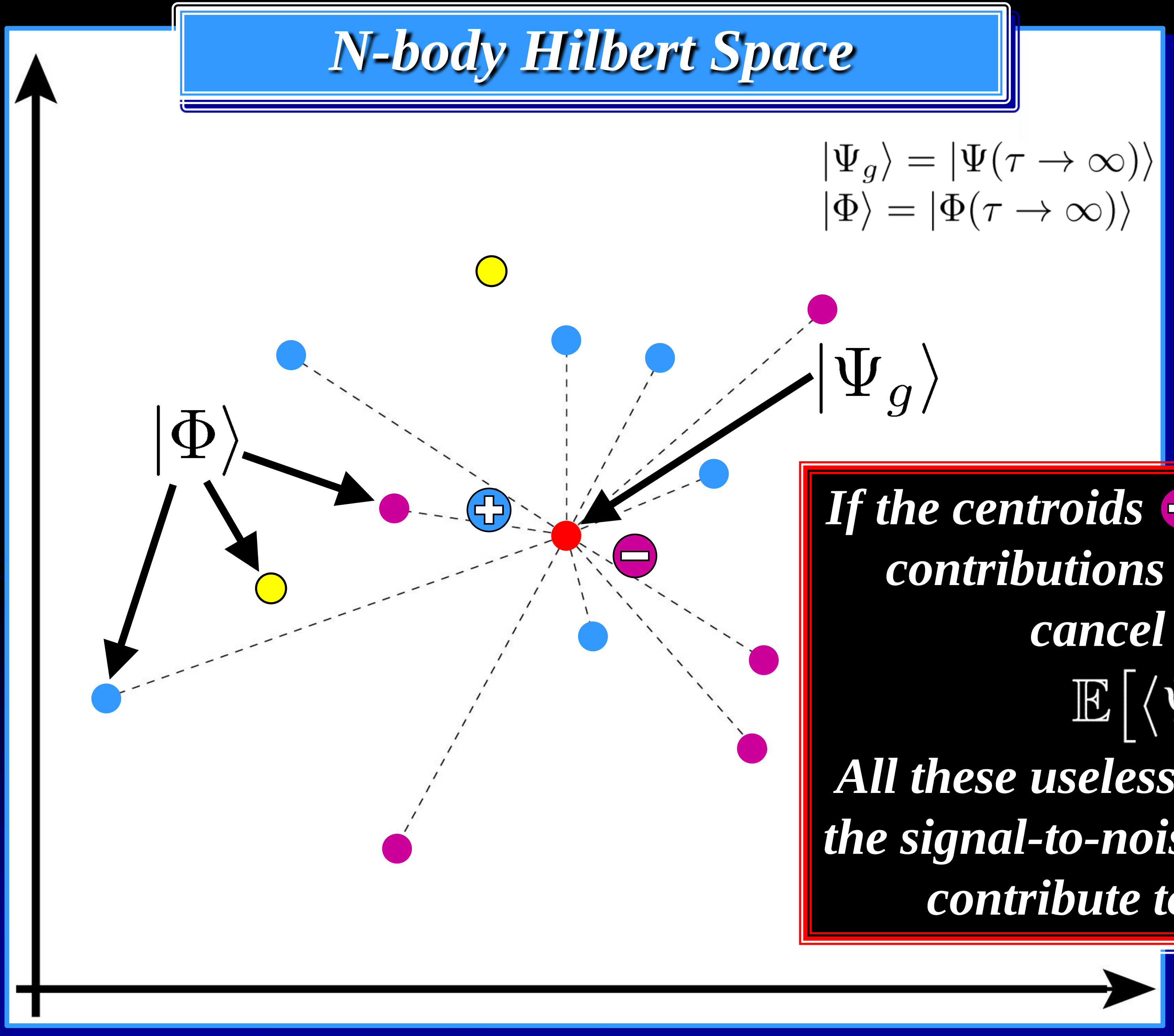
$g_p^s = 5.586\ \ ;\ g_p^l = 1.030$

The Sign Problem



- $\langle \Psi_g | \Phi \rangle > 0$
- $\langle \Psi_g | \Phi \rangle < 0$
- $\langle \Psi_g | \Phi \rangle = 0$

The Sign Problem



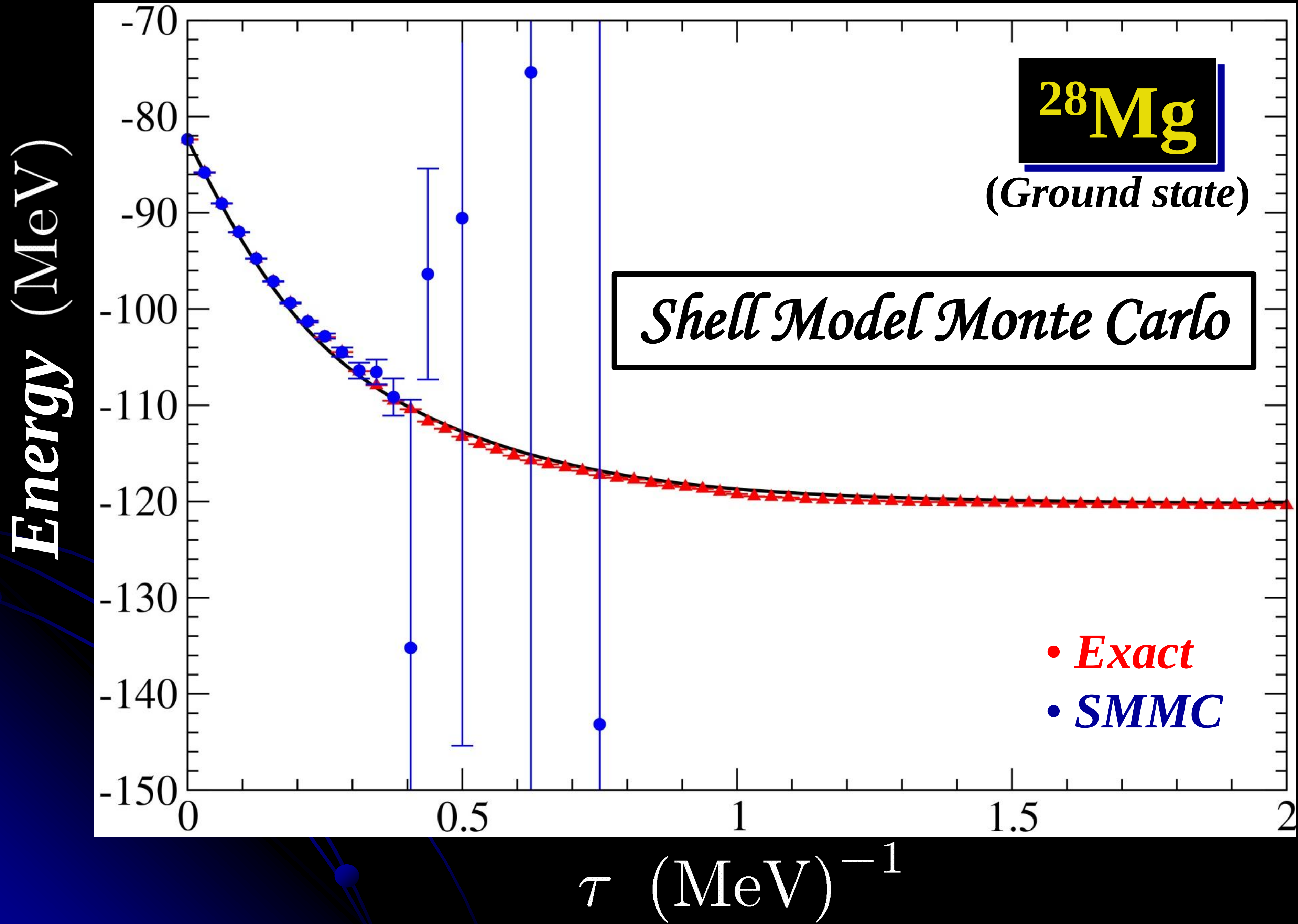
- $\langle \Psi_g | \Phi \rangle > 0$
- $\langle \Psi_g | \Phi \rangle < 0$
- $\langle \Psi_g | \Phi \rangle = 0$

If the centroids ⊖ and ⊕ are merged, the contributions of the two populations cancel each other out:

$$\mathbb{E}\big[\langle \Psi_g | \Phi \rangle\big] = 0 .$$

All these useless trajectories just degrade the signal-to-noise ratio because they only contribute to the statistical error

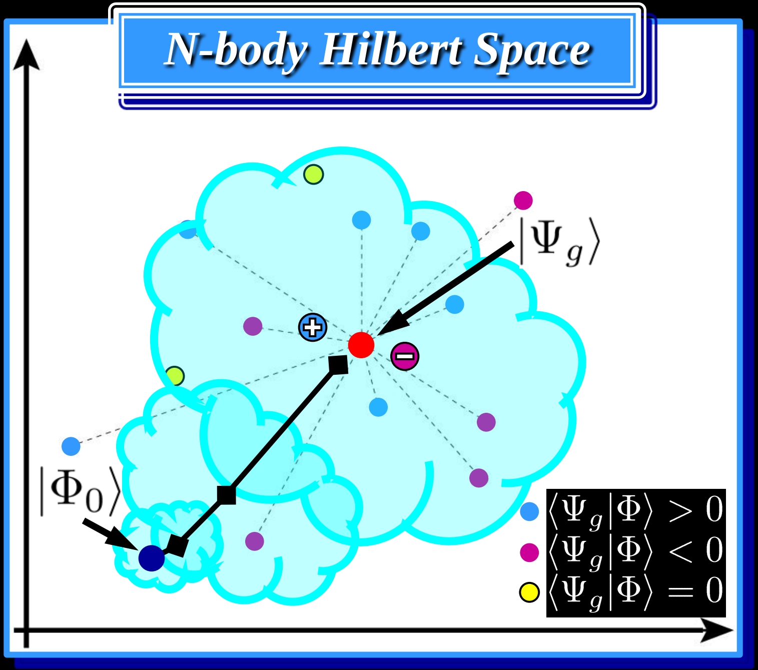
The Sign Problem



Stoitcheva *et al.*, *nucl-th*/0708,2945 (2007)

effective interaction: USD

The Sign Problem

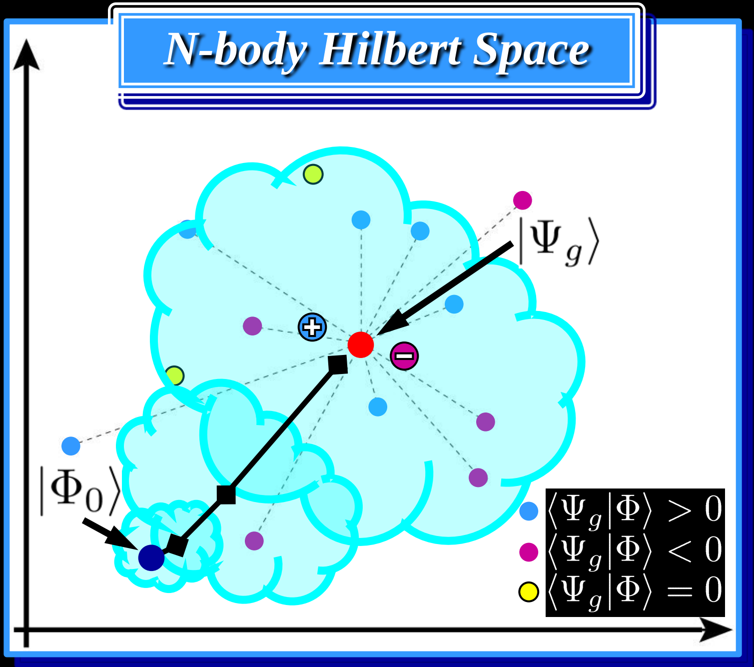


$$\langle\Psi_g|\Phi(\tau_0)\rangle = 0 \Longrightarrow \langle\Psi_g|\,\mathrm{e}^{-(\tau-\tau_0)\hat{H}}|\Phi(\tau_0)\rangle = 0$$

$$\Longrightarrow \forall\tau > \tau_0\,,\; \mathbb{E}\big[\langle\Psi_g|\Phi(\tau)\rangle\big] = 0$$

The resulting walkers can be divided into a population ● and a population ● having exactly opposite contributions

The Sign Problem



$$\langle\Psi_g|\Phi(\tau_0)\rangle = 0 \longrightarrow \langle\Psi_g|\,\mathrm{e}^{-(\tau-\tau_0)\hat{H}}|\Phi(\tau_0)\rangle = 0$$

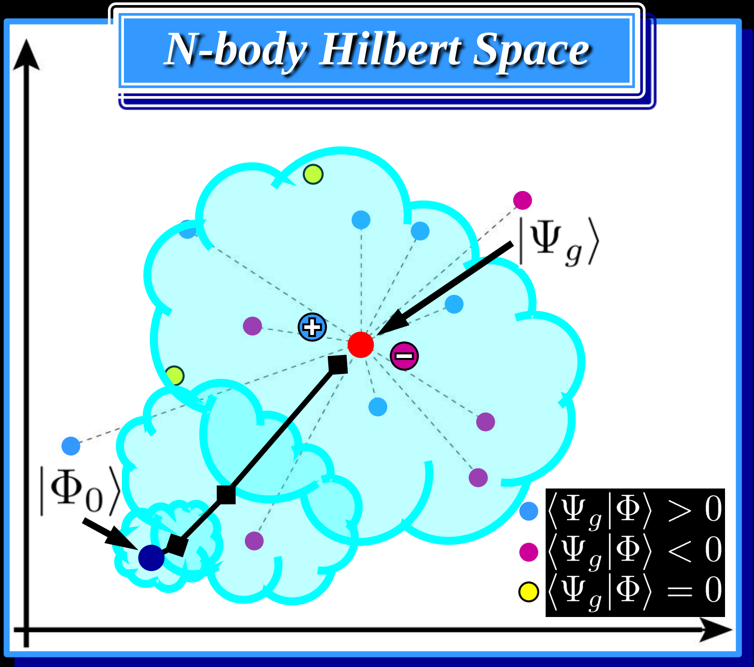
$$\Rightarrow \forall\tau > \tau_0\,,\ \mathbb{E}\big[\langle\Psi_g|\Phi(\tau)\rangle\big] = 0$$

The resulting walkers can be divided into a population ● and a population ● having exactly opposite contributions

Finally, the sign problem can be controlled by imposing :

$$\forall\tau \quad \boxed{\langle\Psi_g|\Phi(\tau)\rangle > 0}$$

The Sign Problem



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The resulting walkers can be divided into a population ● *and a population* ● *having* ***exactly opposite*** *contributions*

Finally, the sign problem can be controlled by imposing :

$$\forall\tau \quad \boxed{\langle\Psi_T|\Phi(\tau)\rangle > 0}$$

Selection with a trial state

Standard approximation used in the nuclear **ab initio** *calculations and in condensed matter physics*

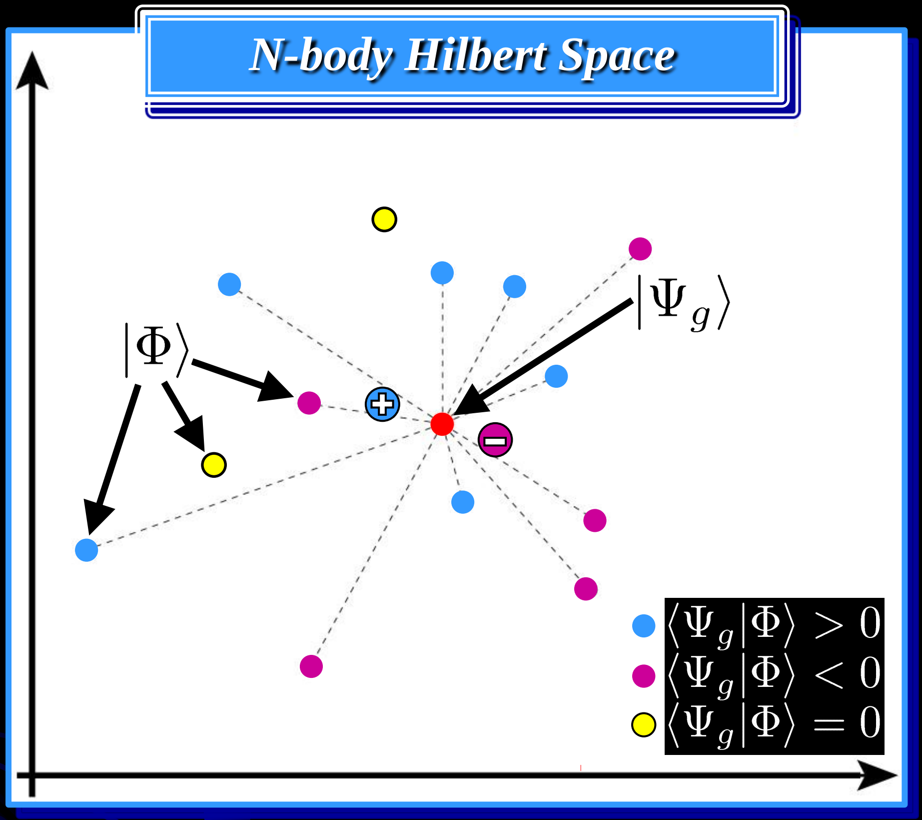
Constrained Path AFQMC

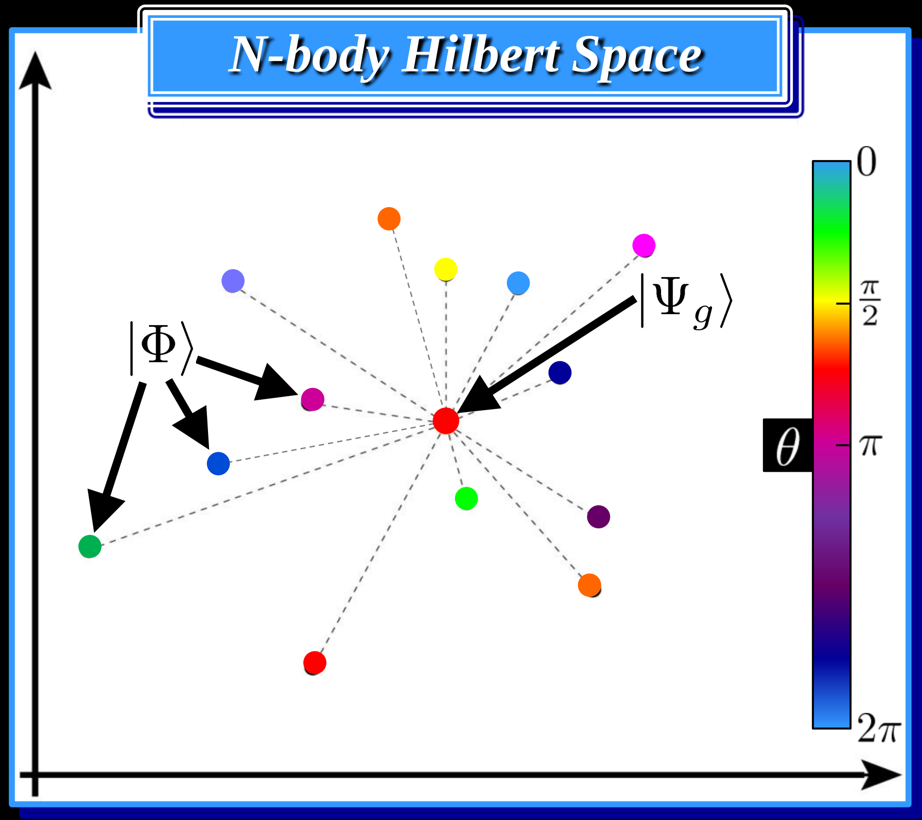
S. Zhang, J. Carlson, J.E. Gubernatis, *PRL* 74,3652 (1995)

Fixed-Node DMC,GFMC

D.M. Ceperley, B. Alder, *PRL* 45,566 (1980)

From the Sign Problem to the Phase Problem





Sign Problem

$$\langle\Psi_g|\Phi\rangle = \pm|\langle\Psi_g|\Phi\rangle|$$

Constrained Path AFQMC

Fixed-Node DMC, GFMC

Phase Problem

$$\langle\Psi_g|\Phi\rangle = |\langle\Psi_g|\Phi\rangle|\, e^{i\theta}$$

Phaseless AFQMC

S. Zhang, H. Krakauer, *PRL* 90,1336401 (2003)

The Phaseless Approximation

$$\boxed{E_g \underset{\tau\to\infty}{=} \frac{\langle\Psi_T|\hat{H}\,\mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle}{\langle\Psi_T|\,\mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle} = \frac{\mathbb{E}[P(\tau)\mathcal{E}(\tau)]}{\mathbb{E}[P(\tau)]}}$$

where $\mathcal{E}(\tau) = \dfrac{\langle\Psi_T|\hat{H}|\Phi(\tau)\rangle}{\langle\Psi_T|\Phi(\tau)\rangle}$ ***is the "local energy"***

The Phaseless Approximation

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where $\mathcal{E}(\tau) = \dfrac{\langle \Psi_T | \hat{H} | \Phi(\tau) \rangle}{\langle \Psi_T | \Phi(\tau) \rangle}$ *is the "local energy"*

Sign Problem

$$\langle \Psi_g | \Phi \rangle = \pm |\langle \Psi_g | \Phi \rangle|$$

Constrained Path AFQMC

$$P_{\mathrm{cp}}(\tau)$$

$$\downarrow$$

$$|P_{\mathrm{cp}}(\tau)| \max\{0, \mathrm{sign}(\langle \Psi_T | \Phi(\tau) \rangle)\}$$

Phase Problem

$$\langle \Psi_g | \Phi \rangle = |\langle \Psi_g | \Phi \rangle| \, \mathrm{e}^{\mathrm{i}\theta}$$

Phaseless AFQMC

$$P_{\mathrm{Ph}}(\tau)$$

$$\downarrow$$

$$\boxed{|P_{\mathrm{Ph}}(\tau)| \max\{0, \Re(\langle \Psi_T | \Phi(\tau) \rangle)\}}$$

The Phaseless Approximation

$$\boxed{E_g \underset{\tau\to\infty}{=} \frac{\langle\Psi_T|\hat{H}\,\mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle}{\langle\Psi_T|\,\mathrm{e}^{-\tau\hat{H}}|\Phi_0\rangle} = \frac{\mathbb{E}[P(\tau)\mathcal{E}(\tau)]}{\mathbb{E}[P(\tau)]}}$$

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Phase Problem

$$\langle\Psi_g|\Phi\rangle = |\langle\Psi_g|\Phi\rangle|\,\mathrm{e}^{\mathrm{i}\theta}$$

Phaseless AFQMC

$$P_{\mathrm{Ph}}(\tau)$$

$$\downarrow$$

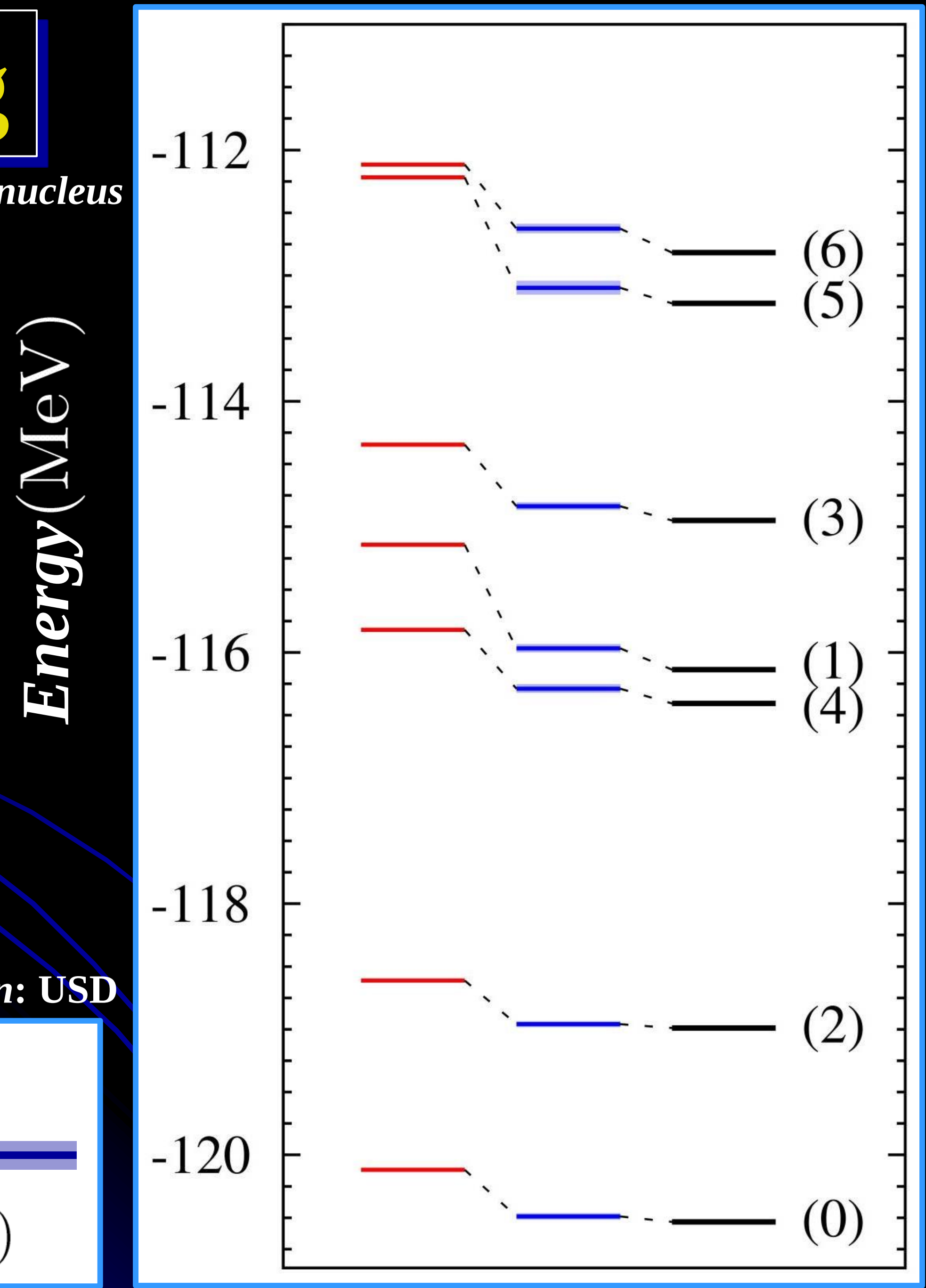
$$\boxed{|P_{\mathrm{Ph}}(\tau)|\max\{0,\Re(\langle\Psi_T|\Phi(\tau)\rangle)\}}$$

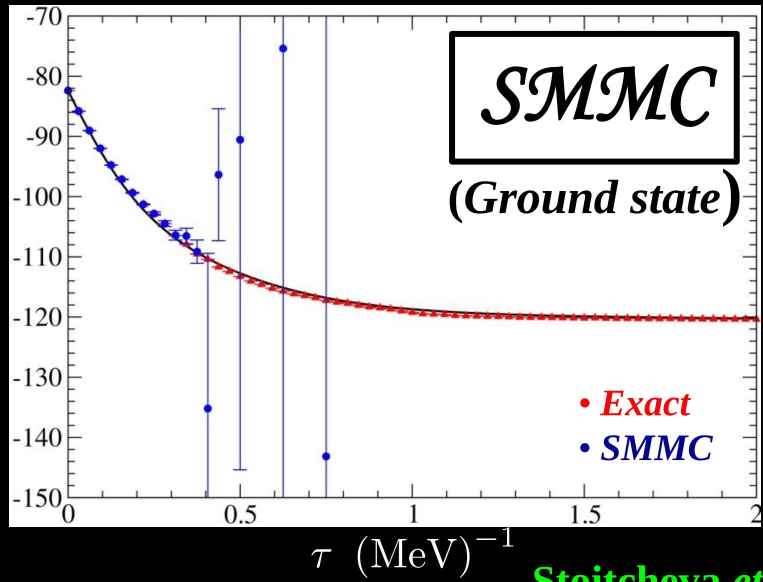
To obtain the "yrast spectroscopy" of nuclei ⇒ $\boxed{|\Psi_T\rangle = |\Psi_{JM}\rangle}$ *The PHF method provides a trial AND an intial wavefunction for each spin*

QMC: *First results*

^{28}Mg

Even-even sd-shell *nucleus*





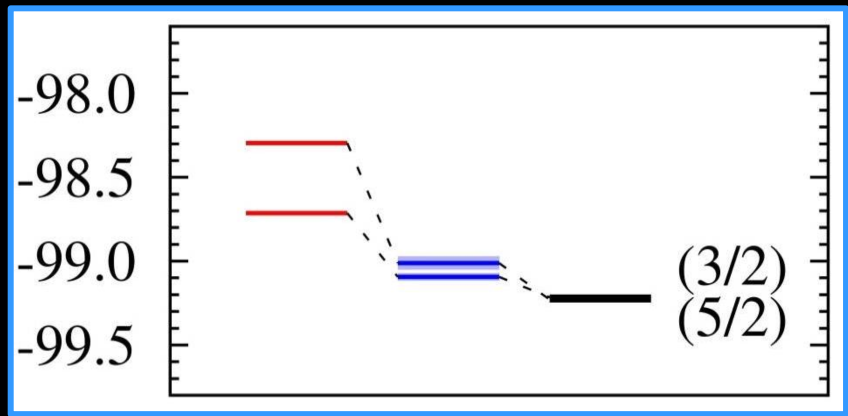
Stoitcheva *et al*.

Effective interaction: USD

- ***PHF***
- ***QMC***
- ***Exact*** (J)

^{27}Na

Odd-mass sd-shell *nucleus*



Conclusions & Perspectives

<u>*Objective*</u> : *The "yrast spectroscopy" of nuclei through the Shell Model* **via** *a stochastic reformulation of the Schrödinger equation*

<u>*Method*</u> :

<u>*Results*</u> :

<u>*Perspectives*</u> :

Conclusions & Perspectives

Objective **:** ***The "yrast spectroscopy" of nuclei through the Shell Model*** **via** ***a stochastic reformulation of the Schrödinger equation***

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Perspectives :

- *Calculations for* **fp**-*shell nuclei* (*not possible at the LPC*);
- *The pairing correlations are stochastically contained within the Brownian motion of the walkers*:

  ↳ *Take them into account directly in the ansatz by propagating Bogoliubov quasiparticle vacua.*

Thank you for your attention

Workshop: "Stochastic Schrödinger Equations"

Dec. 06-07, 2011

CEA/SPhN, Orme des Merisiers, Gif-sur-Yvette

Jérémy Bonnard